



ELSEVIER

Computer Physics Communications 91 (1995) 345-347

---

---

Computer Physics  
Communications

---

---

## Author index to volume 91

Antosiewicz, J., see J.D. Madura	91 (1995) 57
Bagheri, B., see J.D. Madura	91 (1995) 57
Berendsen, H.J.C., D. van der Spoel and R. van Drunen, GROMACS: A message-passing parallel molecular dynamics implementation	91 (1995) 43
Briggs, J.M., see J.D. Madura	91 (1995) 57
Caldwell, J.W., see D.A. Pearlman	91 (1995) 1
Case, D.A., see D.A. Pearlman	91 (1995) 1
Cheatham III, T.E., see D.A. Pearlman	91 (1995) 1
Chow, K.-H. and D.M. Ferguson, Isothermal-isobaric molecular dynamics simulations with Monte Carlo volume sampling	91 (1995) 283
Daggett, V., see M. Levitt	91 (1995) 215
Dalke, A., see M. Nelson	91 (1995) 111
Dauber-Osguthorpe, P., see A.P. Lemon	91 (1995) 97
Davis, M.E., see J.D. Madura	91 (1995) 57
DeBolt, S., see D.A. Pearlman	91 (1995) 1
Elber, R., A. Roitberg, C. Simmerling, R. Goldstein, H. Li, G. Verkhivker, C. Keasar, J. Zhang and A. Ulitsky, MOIL: A program for simulations of macromolecules	91 (1995) 159
Endo, S., see H. Wako	91 (1995) 233
Ferguson, D., see D.A. Pearlman	91 (1995) 1
Ferguson, D.M., see K.-H. Chow	91 (1995) 283
Gilson, M.K., see J.D. Madura	91 (1995) 57
Gō, N., see H. Wako	91 (1995) 233
Goldstein, R., see R. Elber	91 (1995) 159
Goodfellow, J.M., W.R. Pitt, O.S. Smart and M.A. Williams, New methods for the analysis of the protein-solvent interface	91 (1995) 321
Guilbert, C., D. Perahia and L. Mouawad, A method to explore transition paths in macromolecules. Applications to hemoglobin and phosphoglycerate kinase	91 (1995) 263
Gursoy, A., see M. Nelson	91 (1995) 111
Hirshberg, M., see M. Levitt	91 (1995) 215
Humphrey, W., see M. Nelson	91 (1995) 111
Hünenberger, P.H., see W.F. van Gunsteren	91 (1995) 305

Ilin, A., see J.D. Madura	91 (1995) 57
Kale, L., see M. Nelson	91 (1995) 111
Keasar, C., see R. Elber	91 (1995) 159
Keiner, V., see G.R. Kneller	91 (1995) 191
Kneller, G.R., V. Keiner, M. Kneller and M. Schiller, <i>nMOLDYN</i> : A program package for a neutron scattering oriented analysis of molecular dynamics simulations	91 (1995) 191
Kneller, M., see G.R. Kneller	91 (1995) 191
Kollman, P., see D.A. Pearlman	91 (1995) 1
Kufrin, R., see M. Nelson	91 (1995) 111
Lavery, R., K. Zakrzewska and H. Sklenar, <i>JUMNA</i> (Junction minimisation of nucleic acids)	91 (1995) 135
Lemon, A.P., P. Dauber-Osguthorpe and D.J. Osguthorpe, <i>FOCUS</i> : a molecular dynamics analysis program. New features for the characterisation of lipid bilayers and solvated systems	91 (1995) 97
Levitt, M., M. Hirshberg, R. Sharon and V. Daggett, Potential energy function and parameters for simulations of the molecular dynamics of proteins and nucleic acids in solution	91 (1995) 215
Li, H., see R. Elber	91 (1995) 159
Luty, B.A., see J.D. Madura	91 (1995) 57
McCammon, J.A., see J.D. Madura	91 (1995) 57
Madura, J.D., J.M. Briggs, R.C. Wade, M.E. Davis, B.A. Luty, A. Ilin, J. Antosiewicz, M. K. Gilson, B. Bagheri, L.R. Scott and J.A. McCammon, Electrostatics and diffusion of molecules in solution: simulations with the University of Houston Brownian Dynamics program	91 (1995) 57
Mark, A.E., see W.F. van Gunsteren	91 (1995) 305
Micu, A.M. and J.C. Smith, <i>SERENA</i> : a program for calculating X-ray diffuse scattering intensities from molecular dynamics trajectories	91 (1995) 331
Mouawad, L., see C. Guillet	91 (1995) 263
Nagayama, K., see H. Wako	91 (1995) 233
Nelson, M., W. Humphrey, R. Kufrin, A. Gursoy, A. Dalke, L. Kale, R. Skeel and K. Schulten, <i>MDScope</i> —a visual computing environment for structural biology	91 (1995) 111
Osguthorpe, D.J., see A.P. Lemon	91 (1995) 97
Pearlman, D.A., D.A. Case, J.W. Caldwell, W.S. Ross, T.E. Cheatham III, S. DeBolt, D. Ferguson, G. Seibel and P. Kollman, <i>AMBER</i> , a package of computer programs for applying molecular mechanics, normal mode analysis, molecular dynamics and free energy calculations to simulate the structural and energetic properties of molecules	91 (1995) 1
Perahia, D., see C. Guillet	91 (1995) 263
Perahia, D., see T. Simonson	91 (1995) 291
Pettitt, B.M., see P.E. Smith	91 (1995) 339
Pitt, W.R., see J.M. Goodfellow	91 (1995) 321
Roitberg, A., see R. Elber	91 (1995) 159
Ross, W.S., see D.A. Pearlman	91 (1995) 1
Roux, B., The calculation of the potential of mean force using computer simulations	91 (1995) 275

Schiller, M., see G.R. Kneller	91 (1995) 191
Schulten, K., see M. Nelson	91 (1995) 111
Scott, L.R., see J.D. Madura	91 (1995) 57
Seibel, G., see D.A. Pearlman	91 (1995) 1
Sharon, R., see M. Levitt	91 (1995) 215
Simmerling, C., see R. Elber	91 (1995) 159
Simonson, T. and D. Perahia, Dielectric properties of proteins from simulations: tools and techniques	91 (1995) 291
Skeel, R., see M. Nelson	91 (1995) 111
Sklenar, H., see R. Lavery	91 (1995) 135
Smart, O.S., see J.M. Goodfellow	91 (1995) 321
Smith, J.C., see A.M. Micu	91 (1995) 331
Smith, P.E., see W.F. van Gunsteren	91 (1995) 305
Smith, P.E. and B.M. Pettitt, Efficient Ewald electrostatic calculations for large systems	91 (1995) 339
Tironi, I.G., see W.F. van Gunsteren	91 (1995) 305
Ulitsky, A., see R. Elber	91 (1995) 159
Van Belle, D. and S.J. Wodak, Extended Lagrangian formalism applied to temperature control and electronic polarization effects in molecular dynamics simulations	91 (1995) 253
Van Drunen, R., see H.J.C. Berendsen	91 (1995) 43
Van der Spoel, D., see H.J.C. Berendsen	91 (1995) 43
Van Gunsteren, W.F., P.H. Hünenberger, A.E. Mark, P.E. Smith and I.G. Tironi, Computer simulation of protein motion	91 (1995) 305
Verkhivker, G., see R. Elber	91 (1995) 159
Wade, R.C., see J.D. Madura	91 (1995) 57
Wako, H., S. Endo, K. Nagayama and N. Gō, FEDER/2: program for static and dynamic conformational energy analysis of macro-molecules in dihedral angle space	91 (1995) 233
Williams, M.A., see J.M. Goodfellow	91 (1995) 321
Wodak, S.J., see D. Van Belle	91 (1995) 253
Zakrzewska, K., see R. Lavery	91 (1995) 135
Zhang, J., see R. Elber	91 (1995) 159